

Pentafluoropropionic acid
422-64-0 | DTXSID8059970

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.21 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.85e-01

Confidence level: 5.22e-01

Nearest Neighbors from the Training Set

Image not found

Acetic acid, trifluoro-

Measured: 8.77

Predicted: 4.36

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Fluopropanate-sodium

Measured: 1.31e-01

Predicted: 4.65e-01

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2,2,2-Trifluoroethanol

Measured: 10.0

Predicted: 6.34

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1,1,1-Trifluoro-2-propanol

Measured: 2.04

Predicted: 2.45

Image not found

Acetic acid, difluoro-

Measured: 10.4

Predicted: 8.06